cis-1,2,3,4,4a,9a-Hexahydrodibenzothiophene

Inchi: InChI=1S/C12H14S/c1-3-7-11-9(5-1)10-6-2-4-8-12(10)13-11/h1,3,5,7,10,12H,2,4,6,8H2/t
InchiKey: VKFAAUDUBPEOMC-NUHJPDEHSA-N
Formula: C12H14S
SMILES: c1ccc2c(c1)SC1CCCCC21
Mol. weight [g/mol]: 190.31

Physical Properties

Property code	Value	Unit	Source
gf	302.20	kJ/mol	Joback Method
hf	118.75	kJ/mol	Joback Method
hfus	18.32	kJ/mol	Joback Method
hvap	51.05	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.819		Crippen Method
mcvol	150.810	ml/mol	McGowan Method
pc	3173.97	kPa	Joback Method
rinpol	271.39		NIST Webbook
rinpol	271.39		NIST Webbook
tb	571.20	K	Joback Method
tc	826.72	K	Joback Method
tf	379.75	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	367.55	J/mol×K	571.20	Joback Method
cpg	386.56	J/mol×K	613.79	Joback Method
cpg	403.99	J/mol×K	656.37	Joback Method
cpg	419.98	J/mol×K	698.96	Joback Method
cpg	434.68	J/mol×K	741.55	Joback Method
cpg	448.23	J/mol×K	784.13	Joback Method
cpg	460.78	J/mol×K	826.72	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R15383&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume